NUMERICAL CONSTRUCTIONS OF PERTURBATION SERIES IN QUANTUM MECHANICS

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Abstract

Our several recent improvements of the current textbook (so called Rayleigh-Schrödinger) perturbative representation of bound states are reviewed. They were all inspired by an adaptive re-split $H(\lambda) = H^{(0)} + \lambda\, H^{(1)}$ of the Hamiltonian. Their feasibility is facilitated by the use of nonstandard bases and by the flexibility of normalization of the wave functions $\psi(\lambda)$.

1 Introduction

Anharmonic oscillators often serve as a methodical laboratory in quantum mechanics [1]. Schrödinger equation which determines their bound states is, in the time-independent case, an elliptic partial differential boundary-value problem, currently analysed by the variational or perturbation techniques. In the latter context, one of the most transparent illustrations of the implementation and of the efficiency of the method is provided by the elementary one-dimensional quartic example

$$-\frac{d^2}{dx^2}\,\psi(x)+V(x)\,\psi(x)=E\,\psi(x) \tag{1}$$

with boundary conditions $\psi(\pm\infty)=0$, one-parametric family of potentials $V(x)=x^2+\lambda\,x^4$ and with the so called Rayleigh-Schrödinger formal-series solution

$$\begin{aligned}\psi(x)&=\psi^{(0)}(x)+\lambda\;\psi^{(1)}(x)+\lambda^2\psi^{(2)}(x)+\ldots,\\ E&=E^{(0)}+\lambda E^{(1)}+\lambda^2E^{(2)}+\ldots\;.\end{aligned} \tag{2}$$

The example nicely illustrates the main merits of the Rayleigh-Schrödinger approach (feasibility, numerical efficiency near $\lambda\approx 0$) as well as several of its most characteristic difficulties.

In particular, the mere asymptotic and, hence, divergent-series character of the anharmonic-oscillator "solutions" (2) divided the physics community into supporters and opponents of the perturbative considerations. During the last thirty years of development, the former group definitely prevailed. In what follows, an illustration of the latter tendency will be presented via a review of some of a few of my own recent innovations of the general perturbation formalism.

2 Formalisms which do not need the unperturbed basis

One of the most important merits of perturbative considerations lies in their analytic treatment of certain parameters and in their enormous (though not always fully appreciated) formal flexibility. In this sense, there exists an ample variety of alternatives to the standard textbook representation of wave functions (2) in the (orthonormalized) basis $\{ |n\rangle \}$ of the $\lambda = 0$ eigenstates of $H(0)$,

$$\psi^{(k)}(x) = \sum_{n=0}^{\infty} \langle x|n\rangle \, p_n^{(k)} \ . \tag{3}$$

In this review of my own contributions to this effort I would like to mention the representations of wave functions

- employing the Runge-Kutta-like discretizations of the domain of coordinates, both in one [2] and more [3] spatial dimensions;
- using the bases with nontrivial orthogonality: Sturmianic [4], complexified [5] etc;
- switching to techniques which do not need any scalar product at all and comprise the Taylor-like expansions in the origin [6] as well as near infinity [7].

All these alterations of eq. (3) are able to simplify, first of all, the evaluation of the matrix elements of the perturbation Hamiltonians $H^{(k)}$.

In this context one should also mention a closely related trick of working with the so called "whacko", order-dependent auxiliary Hamiltonians and bases as employed, e.g., in the non-linear context of the so called delta-expansions [8].

3 Formalisms with non-diagonal propagators

In the purely technical sense, the appeal of the textbook perturbative considerations may be traced back to their frequent use of the fully diagonalized zero-order models $H^{(0)}$. In practice, an availability of such a type of an approximant is in fact very rare. At the same time, people are often seduced by the extremely transparent formulae obtainable due to the diagonality of the necessary (so called unperturbed) auxiliary propagators R (schematically: $R \sim (H^{(0)} + const)^{-1}$).

Here, we would like to emphasize, as one of the basic ideas of the present review, that the construction of the perturbation series (2) does not necessarily require a *complete* solvability/solution of the Schrödinger equation

$$H(\lambda)\,|\psi(\lambda)\rangle = E(\lambda)\,|\psi(\lambda)\rangle \tag{4}$$

at *any particular* (usually, zero) value of the auxiliary parameter $\lambda = \lambda^{(0)}$.

There exists, in fact, a balance between the strongly redundant [9] requirements of a *complete* solution of the zero-order problem

$$(H(\lambda^{(0)}) - E(\lambda^{(0)}))|\psi(\lambda^{(0)})\rangle = 0 \tag{5}$$

and the related enhancement of economy of the solution of the first-order problem

$$(H(\lambda^{(0)}) - E(\lambda^{(0)}))|\psi^{(1)}\rangle + (H^{(1)} - E^{(1)})|\psi(\lambda^{(0)})\rangle = 0 \tag{6}$$

and of its further higher-order descendants

$$(H(\lambda^{(0)}) - E(\lambda^{(0)}))|\psi^{(k)}\rangle = E^{(k)}|\psi(\lambda^{(0)})\rangle + |\tau\rangle. \tag{7}$$

One has to defend a compromise and insist on the obvious observation that the inter-related pair (or rather multiplet of the $K+1$ linear operator equations) (5) and (7),

i.e., the set of the linear operator equations

$$A(E^{(0)})\vec{x} = 0, \qquad A(E^{(0)})\vec{y}^{(k)} = \vec{b}^{(k-1)}(E^{(k)}), \qquad k = 1, 2, \ldots, K \tag{8}$$

should be considered as a single, unseparated (and, in general, purely numerical) problem of determination of the unknown quantities $\vec{x}$, $E^{(k-1)}$ and $\vec{y}^{(k)}$.

In this sense, one can accept various computational strategies. In a way depending on our deeper insight in the structure of the operator A and in its explicit computational representation, one could propose the use of some "surviving" simplifications offered, e.g.,

- by any form of an *incomplete* analytic solvability of the zero order equation (5); whenever available, such a solvability is still able to simplify the computations significantly [10];

- by any algebraization of the Schrödinger eq. (4); it provides a new origin of perturbative constructions as exemplified by the non-variational recipe of ref. [11] or, in the much more numerical context, by the algorithms of ref. [12].

In all the above-mentioned examples a key role is played by the band-matrix structure of the unperturbed Hamiltonian. Also the sparse-matrix structure of its perturbative "user-friendly" components can make the resulting solution of the whole set of equations (8) very straightforward and comfortably feasible. Such a construction proceeds in fact along the same lines (and with almost the same ease) as in our introductory anharmonic example, *in spite of the fact* that the unperturbed propagators themselves remain significantly off-diagonal.

4 Working without the model space projectors

The main price we have to pay for the enhanced flexibility of the above innovated algorithms is that we lose an immediate insight in the structure of the unperturbed problem itself.

Several tricks may help to elucidate this structure, at least, indirectly:

- New attention can be paid to the large but still rigorously terminating cases where, i.a., a new, triple-series formalism has been shown manageable [13];

- More attention can be paid to the optimization of our choice of the zero-order Hamiltonian operator itself. For this purpose, the above-mentioned Runge-Kutta perturbation theory has been combined with an iterative improvement of $H^{(0)}$, e.g., in ref. [14].

- In an active manner, we may get even much further. Thus, controling the mutual methodically relevant relationship between the feasibility of solution of the homogeneous and non-homogeneous parts of the Rayleigh-Schrödinger hierarchy of equations (8) we can introduce also an *ad hoc*, Hartree-Fock-style re-arrangements of many error terms, etc. More technical details about this efficient strategy can be found, e.g., in ref. [15] as well as in the further references listed therein.

One of the main merits of our various modified perturbation prescriptions may be seen in their shared enhanced flexibility and in their consequently recurrent character. Nevertheless, the related algorithms minimizing the distance between $H(\lambda)$ and $H^{(0)}$ also exhibit a serious weak point: By their construction, they would all fail in the (quasi-)degenerate systems. In this context, the most promising development seems

to be represented by the following two different strategies.

- One can get rid of the model space projectors completely. The first attempt in this direction is provided by an inverse-iteration-inspired new scheme of ref. [16].

- One can employ the shooting-like philosophy as implemented in full detail in ref. [17].

Technically, a key problem lies in a preservation of feasibility of evaluation of the separate Rayleigh-Schrödinger perturbation coefficients. In this setting the relaxation of the usual orthogonality of the bases and Hermiticity of the Hamiltonians seems to open an access to many new unperturbed $H^{(0)}$. Simultaneously, a weakening and reduction of the traditional exact solvability requirements opens an access to many new partially or numerically solvable zero-order approximants with an immediate approximative role in realistic models.

5 Outlook

The main common purpose of the present proposal of transition to the semi- or numerical evaluation of corrections lies in the related possibility of a consequent minimization of the absolute magnitude of the perturbation corrections themselves. In this sense, the "size" (whatever it means) of the perturbation Hamiltonian is efficiently suppressed via a weakening of the technical constraints imposed upon its eligible zero-order partners.

We may summarize that the measurable characteristics of various systems in nuclear and atomic physics or quantum chemistry may be fairly well approximated

using some of the reviewed non-standard perturbation methods. They reach beyond the vicinity of the usual exactly solvable zero order models. This significantly extends the domain of applicability of perturbation expansions to many new interesting and comparatively complicated systems.

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